N-Cycloheptyl-N'-phenylurea 19095-79-5 | DTXSID10172606

Model Performance

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Model	I)ata
Widdei	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 291 °C

Global applicability domain: Outside

Local applicability domain index: 2.16e-01

Confidence level: 7.18e-01

Nearest Neighbors from the Training Set

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Diphenylurea Measured: 262 Predicted: 269

Image not found

Benzoic acid, 2-phenylhydrazide

Measured: 314 Predicted: 306

Image not found

N-(4-Bromophenyl)urea

Measured: 260 Predicted: 256

Image not found

Carbaryl Measured: 315 Predicted: 297

Image not found

2-Nitrobenzamide Measured: 317 Predicted: 310